On the spatial and temporal discretization of vertical diffusion in the turbulent planetary boundary layer

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PS14B-2847

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Context: advection-diffusion operator to parameterize unresolved scales in PBLs (and beyond)

The resulting turbulent viscosity/diffusivity K

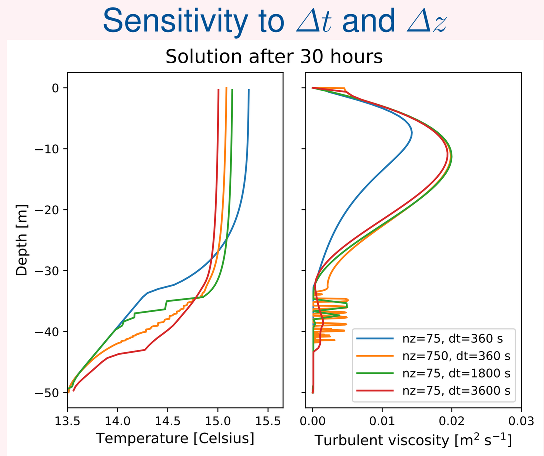
$\to$ strongly varies spatially, i.e. large values of $\frac{h(\partial_z K)}{K}$

$\to$ depends nonlinearly on model variables

$\to$ induces stiffness, i.e. large $\sigma^{(2)} = \frac{K \Delta t}{h^2}$

Usual approach: use of (semi)-implicit temporal schemes with 2nd-order FD discretization

Sensitivity to Δt and Δz



Single-column exp. (Wind-induced deepening of BL)

What could be wrong with 2nd-order in space ?

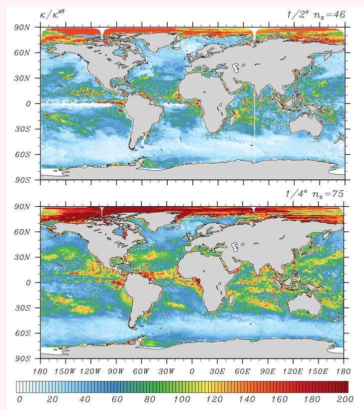
- With $\mathrm{Pe}^{(n)} = \frac{h^n \partial_z^n K}{K} \neq 0,\ n \geq 1$

$$\partial_z (K\partial_z\phi)_k^{(\mathrm{C2})} = \partial_z(K\partial_z\phi)_k + \frac{1}{24}\partial_z\left(K\left[\mathrm{Pe}^{(2)}\partial_z\phi + 2\Delta z \mathrm{Pe}^{(1)}\partial_z^2\phi + 2\Delta z^2\partial_z^3\phi\right]\right) + \mathcal{O}(\Delta z^4)$$

What could be wrong with (semi)-implicit scheme in time ?

- Lack of monotonic damping / Inexact damping for large $\sigma^{(2)}$
- $\mathcal{O}(\Delta t)$ errors in coupling with physical parameterizations

Maps of $\frac{K}{K^{\mathrm{num}}}$ from realistic simulations [Lemarié et al., 2015]



- K^{num} is the diffusivity in the continuous equation with same damping as the numerical damping
- $K/K^{\mathrm{num}} \gg 1 \Rightarrow$ the damping seen by the model is smaller than the theoretical damping ($\sigma^{(2)} = \sigma^{\mathrm{mld}}$, $\theta = \frac{2\pi}{N_{\mathrm{mld}}}$).

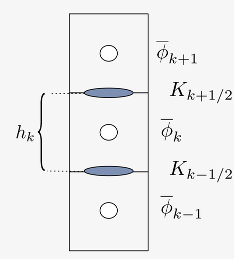
Objectives:

- Have a better control of numerical sources of error independently from the physical principles of the subgrid scheme
- Ensure the consistency between the parameterization and the resolved fluid dynamics (e.g. for air-sea B.C. & $K(z)$ computation)

1 - Spatial discretization

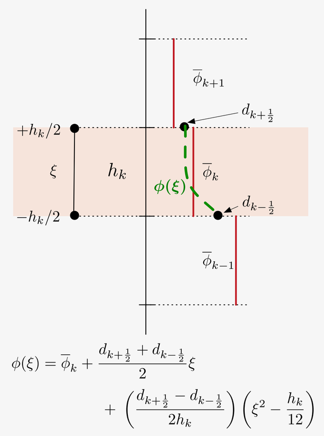
Constraints

- limit ourselves to tridiagonal linear problems
- possibility to have a joint treatment of vertical advection and diffusion
- allow a finite-volume interpretation



Possible alternatives

- Exponential Compact scheme, e.g. [Tian & Dai, 2007]
  - $\to$ Specifically designed for accuracy with large Peclet numbers
- Padé compact finite volume discretization



General form of the discretization

$$\partial_z(K\partial_z\phi) = \frac{K_{k+1/2}d_{k+1/2} - K_{k-1/2}d_{k-1/2}}{h_k}, \qquad d_{k+1/2} = (\partial_z\phi)_{k+1/2}$$

for standard discretization: $d_{k+1/2} = (\phi_{k+1} - \phi_k)/h_{k+1/2}$ (h : vertical layers thickness)

Compact Padé Finite Volume methods, e.g. [Kobayashi, 1999]

Unknowns : derivatives $d_{k+\frac{1}{2}}$ on cell interfaces, for $m, n \in \mathcal{N}$

$$\sum_{i=1}^{m}\alpha_i d_{k+\frac{1}{2}-i} + d_{k+\frac{1}{2}} + \sum_{i=1}^{m}\alpha_i d_{k+\frac{1}{2}+i} = \frac{1}{h}\left(\sum_{j=1}^{n}\gamma_j\overline{\phi}_{k+j} - \sum_{j=1}^{n}\gamma_j\overline{\phi}_{k-j+1}\right)$$

- For $(m,n) = (1,1)$: $\alpha_1 d_{k-\frac{1}{2}} + d_{k+\frac{1}{2}} + \alpha_1 d_{k+\frac{3}{2}} = \gamma_1\left(\frac{\overline{\phi}_{k+1} - \overline{\phi}_k}{h}\right)$

$(\alpha_1, \gamma_1) = \left(\frac{1}{10}, \frac{6}{5}\right)$ $\to$ 4th-order discretization of $d_{k+\frac{1}{2}}$ (for $K = \mathrm{cste}$)

$(\alpha_1, \gamma_1) = \left(\frac{1}{4}, \frac{3}{2}\right)$ $\to$ equivalent to parabolic splines reconstruction.

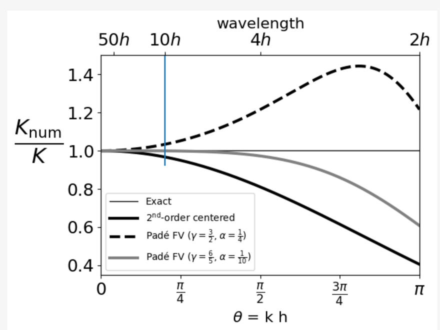


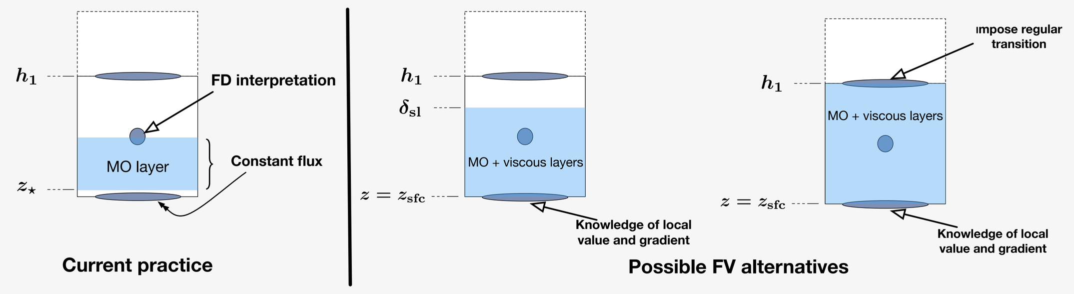
Figure 1: Ratio of numerical vs exact diffusion w.r.t. the normalized wavenumber $\theta = k_z h$ for different spatial discretizations.

- Can be reinterpreted in terms of subgrid reconstruction as parabolic splines
- Flexibility provided by α and γ parameters

2 - Treatment of the boundary condition (Monin-Obukhov consistency)

no-slip boundary condition is never applied in practice

$\to$ replaced by a flux condition consistent with wall laws



Current practice :

$$\begin{cases} \partial_z\left(\kappa|\phi_\star|(z+z_\star)\partial_z\phi\right) = 0 \\ \phi(z_\star) = \chi_{\mathrm{sfc}} \\ \phi(h_1/2) = \phi_1 \end{cases}$$

$$\phi(z) = (\phi_1 - \chi_{\mathrm{sfc}})\left(\frac{\ln\left(\frac{1}{2} + \frac{z}{2z_\star}\right)}{\ln\left(\frac{1}{2} + \frac{h_1}{4z_\star}\right)}\right) + \chi_{\mathrm{sfc}}$$

FV approach with $h_1 = \delta_{\mathrm{sl}}$:

$$\begin{cases} \partial_z\left(\kappa|\phi_\star|(z+z_\star)\partial_z\phi\right) = 0 \\ \phi(z_{\mathrm{sfc}}) = \chi_{\mathrm{sfc}} \\ \phi(h_1) = \phi_{3/2} \end{cases}$$

$$\phi(z) = (\phi_{3/2} - \chi_{\mathrm{sfc}})\left(\frac{\ln\left(1 + \frac{z}{z_\star}\right)}{\ln\left(1 + \frac{h_1}{z_\star}\right)}\right) + \chi_{\mathrm{sfc}}$$

- **Asymptotics :**

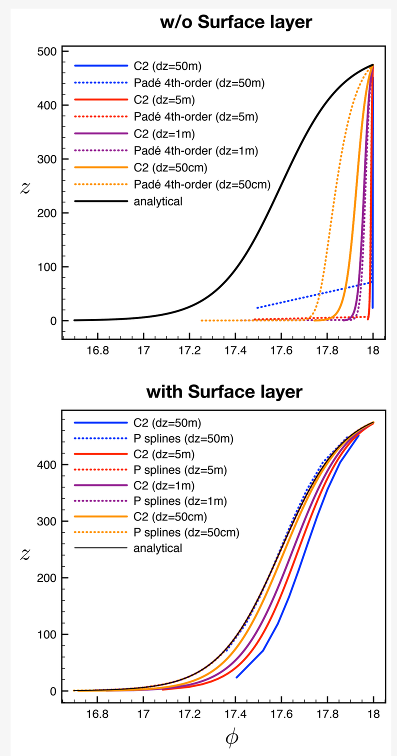
Resolved case (combining the first 2 lines of the matrix)

$$\frac{1}{6}d_{5/2} + \frac{5}{6}d_{3/2} + \frac{1}{2}d_{1/2} = \frac{\overline{\phi}_2 - \chi_{\mathrm{sfc}}}{h}$$

Unresolved case (for $h \to 0$)

$$\frac{1}{6}d_{5/2} + \underbrace{\left(\frac{1}{3} + \left[1 + \frac{h}{2z_\star}\right]\right)d_{3/2}}_{\frac{5}{6}d_{3/2} + \frac{1}{2}d_{1/2}} = \frac{\overline{\phi}_2 - \chi_{\mathrm{sfc}}}{h}$$

Smooth transition between the unresolved and the resolved limit



- **Numerical experiment :**

$$\partial_z\left(K(z)\partial_z\phi\right) = \frac{\partial_z\mathcal{R}}{\rho C_p}, \qquad \phi(0) = \phi_{\mathrm{bot}}, \qquad \phi\left(\frac{19h_{\mathrm{bl}}}{20}\right) = \phi_{\mathrm{top}}$$

3 - Combination with time discretization

Combining Padé type schemes with implicit Euler leads to

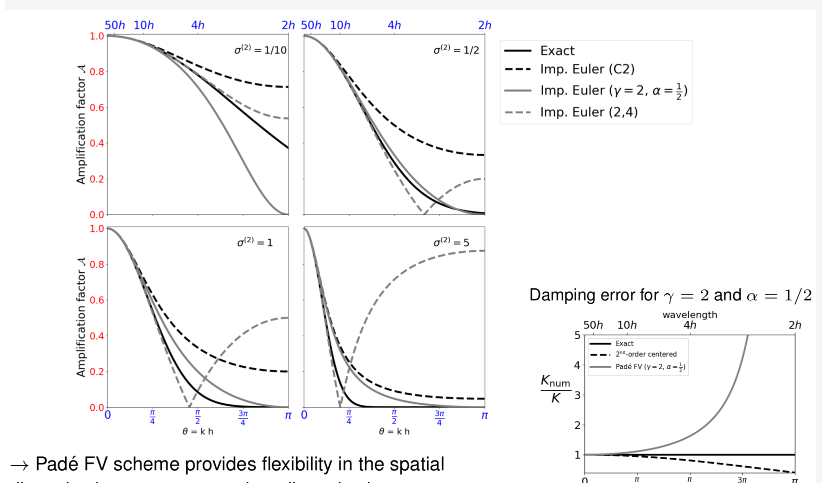
$$\left(\frac{\alpha}{\gamma} - \frac{K_{k+3/2}\Delta t}{h^2}\right)d_{k+3/2}^{n+1} + \left(\frac{1}{\gamma} + 2\frac{K_{k+1/2}\Delta t}{h^2}\right)d_{k+1/2}^{n+1} + \left(\frac{\alpha}{\gamma} - \frac{K_{k-1/2}\Delta t}{h^2}\right)d_{k-1/2}^{n+1} = \frac{\overline{\phi}_{k+1}^n - \overline{\phi}_k^n}{h} + \frac{\Delta t}{h}(\mathrm{rhs}_{k+1} - \mathrm{rhs}_k)$$

- easy to generalize for non-constant grid-size
- The tridiagonal solve provides the flux and not $\overline{\phi}$

Properties for well-behaved numerical solutions

- Unconditional stability
- Monotonic damping (damping increases with increasing wavenumber, i.e. $\partial_\theta\mathcal{A} < 0$)
- Non-oscillatory (i.e. $\mathcal{A} \geq 0$)
- Proper control of grid-scale noise $\forall\sigma^{(2)}$

$\to$ Convergence & stability are often not sufficient



$\to$ Padé FV scheme provides flexibility in the spatial discretization to counteract time discretization errors.

With implicit Euler scheme :

$$\mathcal{A}(\sigma^{(2)}, \theta) = \frac{1 + 2\alpha\cos\theta}{1 + 2\alpha\cos\theta + 4\gamma\sigma^{(2)}(\sin\frac{\theta}{2})^2}$$

- 2nd-order accurate in space : $\alpha = \frac{\gamma - 1}{2}$
- $\forall\gamma \neq 0$, $\partial_\theta\mathcal{A} < 0$: non-oscillatory if $\mathcal{A}(\pi) \geq 0$
- Two possibilities :
  - $\mathcal{A}(\sigma^{(2)}, \pi) = 0 \ \to\ \gamma = 2$
  - 4th-order in space $\to\ \gamma = \frac{6}{5 - 6\sigma^{(2)}}$

4 - Combination with subgrid closure schemes and energetic consistency

For X-equation closures with $X > 0$ a global energy budget can be derived

$$\begin{aligned} \partial_t u - \partial_z(K_m\partial_z u) &= 0 \\ \partial_t b - \partial_z(K_s\partial_z b) &= 0 \end{aligned} \quad\to\quad \begin{aligned} \partial_t\mathrm{KE} - \partial_z(K_m\partial_z\mathrm{KE}) &= -K_m(\partial_z u)^2 = -P \\ \partial_t\mathrm{PE} - \partial_z((-z)K_s\partial_z b) &= \ \ K_s\ \partial_z b \ \ = -B \end{aligned}$$

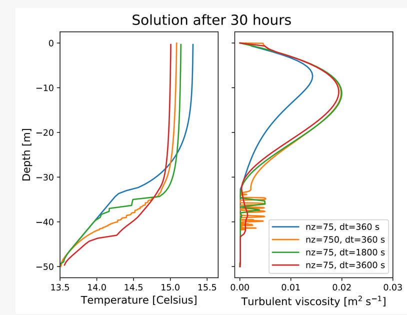
$$\partial_t\mathrm{TKE} - \partial_z(K_e\partial_z\mathrm{TKE}) = P + B - \varepsilon$$

Energy budget in a water column (ignoring the contribution of B.C.) with ε the TKE dissipation:

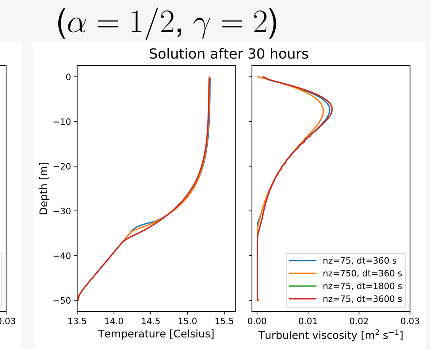
$$E = \int_{z_{\mathrm{bot}}}^{z_{\mathrm{top}}}(\mathrm{KE} + \mathrm{PE} + \mathrm{TKE})dz \quad\to\quad \partial_t E = -\int_{z_{\mathrm{bot}}}^{z_{\mathrm{top}}}\varepsilon dz$$

- The discrete counterpart of it tells you exactly how to discretize forcing terms in the TKE equation
- Numerical experiment: single column with 0-equation closure (KPP, [Large et al., 1994])
  - Use subgrid reconstruction to detect critical Ri-number
  - "Energy consistent" discretization of the Richardson number

Standard approach



Implicit Euler + FV Padé ($\alpha = 1/2$, $\gamma = 2$)



Turbulent Shear and buoyancy production

(methodology of [Burchard 2002])

$$(\partial_z u)_{k+1/2}^2 = d_{k+1/2}^u\left\{\frac{(u_{k+1}^{n+1} + u_{k+1}^n) - (u_k^{n+1} + u_k^n)}{2h_{k+1/2}}\right\}$$

$$(\partial_z b)_{k+1/2} = d_{k+1/2}^b$$

Relevant not only for TKE closure but also for Ri based closure schemes

5 - Summary & Perspectives

Summary

- Padé FV approach provides a good combination of simplicity and flexibility to handle diffusive terms with minimal changes in existing codes
  - Allows a good combination with surface layer param. and existing time-stepping
  - Provides degrees of freedom to mitigate numerical errors in time or to impose desired properties
- Simple single column test (Kato & Phillips) indicates a reduced sensitivity to numerical parameters

Perspectives

- Nonlinear stability
- Extension to mass-flux scheme
- Air-sea interface boundary condition
  - Neutral case $\to$ stratified case
- Single column tests & global ocean simulation
- Add representation of oceanic molecular sublayer + MO layer in the top most oceanic grid box for OA coupling purposes, e.g. [Zeng & Beljaars, 2005]

References